

# Comparison of $M_0$ and $M_1$ for FVP and Bethe methods

Hans Bichsel

December 18, 2008

*e-mail: hbichsel@u.washington.edu*

*Center for Experimental Nuclear Physics and Astrophysics*

*Box 354290 University of Washington*

*Seattle, WA 98195-4290*

## 1 Introduction

In a short review [1] I compared the terms of the B-F and the FVP equations used to calculate the collision cross section differential in energy loss  $E$  (DCCS) for Si. Due to the difference in the approximation for the GOS shown in Fig. 1, there are large differences in two of the terms in the equations, but the difference in the total DCCS is smaller. The effect of the differences can be assessed in the *moments* of the DCCS. They are given by

$$M_\nu(\beta) = \int E^\nu \sigma(E; \beta) dE \quad (1)$$

where  $\beta = v/c$  is the particle speed,  $\sigma(E; \beta)$  the DCCS [1, 2] and  $E$  the energy loss in a collision. It is customary to call  $M_1$  the stopping power, and  $M_0$  the total CCS. The comparison for Si is given in Table 1.

Table 1. Comparison of  $M_0$  and  $M_1$  for B-F and FVP [2].

$\beta\gamma$	$M_0$			$M_1$		
	B-F	FVP	diff%	B-F	FVP	diff%
0.316	30.32	32.78	8.1	2443.7	2465.3	0.9
1.000	6.729	7.175	6.6	578.3	581.8	0.6
3.981	3.952	4.189	6.0	386.1	387.9	0.5
10.000	3.842	4.068	5.9	416.9	418.6	0.4
100.000	3.842	4.066	5.8	503.8	505.4	0.3

The difference in  $M_0$  is quite large for accurate work and should be explored further, especially for gases.

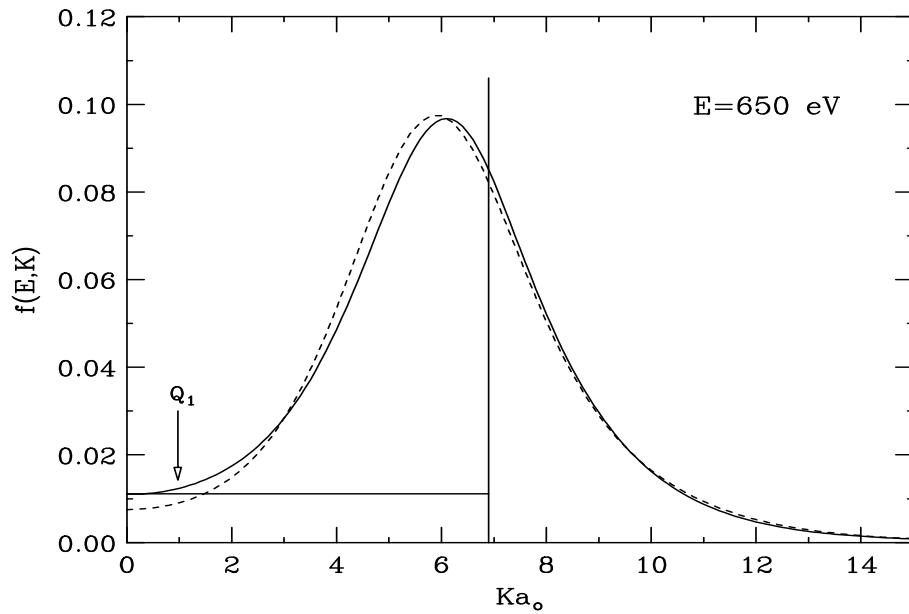


Figure 1: Generalized oscillator strength GOS for Si for an energy transfer  $E = 650$  eV to the 2p-shell electrons [4]. Solid line: calculated with Herman-Skilman potential [5], dashed line: hydrogenic approximation [6]. The horizontal and vertical line define the GOS approximation used in FVP. See Figs. 3-8 in [4] for details.

## 2 Analytic calculation of $M_0$ and $M_1$

I have not implemented the B-F method for gases (No tables of GOS were available, but see [2, 3]). Therefore I compare results of  $M_0$  and  $M_1$  for Ne and Ar with values calculated with analytic

expressions (“Bethe method”) derived in [7, 8, 9, 10]. The Bethe method used to calculate  $M_0 = \sigma_{tot} = \text{CCS}$  is

$$\sigma_{tot} = k_R \left[ S(-1) \left( \ln(2mc^2 \beta^2 \gamma^2 / Ry) - \beta^2 - \ln(c_{tot}) \right) \right] \quad (2)$$

where  $k_R = 2\pi z^2 e^4 Ry / (mc^2 \beta^2)$  and

$$S(\nu) = \int \left( \frac{E}{Ry} \right)^\nu f(E, 0) dE \quad (3)$$

where  $f(E, 0)$  is the dipole oscillator strength. We calculate  $\ln(c_{tot})$  with

$$S(-1) \ln(c_{tot}) = -2 L(-1) + \mathcal{J}_1 - \mathcal{J}_2 \quad (4)$$

where

$$L(\nu) = \int \left( \frac{E}{Ry} \right)^\nu f(E, 0) \ln \frac{E}{Ry} dE. \quad (5)$$

The quantity  $\mathcal{J}_1 - \mathcal{J}_2$  is derived from the generalized oscillator strength (GOS) and for this study is taken from Table I in [9]. The quantities  $S(\nu)$  and  $L(\nu)$  are calculated in the programs BethNe.for and BethAr.for, which are also used for the calculations described in [2, 11].

The *stopping power*  $M_1$  in the Bethe approximation is

$$M_1 = k_R \left[ S(0) \left( \ln(2mc^2 \beta^2 \gamma^2 / Ry) - \beta^2 - \ln I \right) \right] \quad (6)$$

where  $S(0) = Z$ , and  $\ln I = L(0)/S(0)$  is the logarithm of the I-value.<sup>1</sup> It is important to note that no explicit factor derived from the GOS appears here. This is because a sum-rule for the GOS (Eq. 27 in [12]) can be used to calculate  $M_1$ . In the approximation for the GOS described in Fig. 1 the same sum-rule is used to give the factor for the delta-function [1]. Therefore for this GOS model,  $M_1$  is well approximated. For  $M_0$  the quantity  $\mathcal{J}_1 - \mathcal{J}_2$  will not be well approximated with this choice of GOS (but I have not tried to calculate it).

### 3 Numerical calculation of $M_0$ and $M_1$

DCCS  $\sigma(E; \beta)$  are calculated for protons with kinetic energy  $T$  using the *computer-analytic method* with the FVP approximation (FORTRAN program NeSax) [1, 4]. The quantities  $S(\nu)$ ,  $L(\nu)$ , the

---

<sup>1</sup>For 10 MeV protons,  $(\ln(2mc^2 \beta^2 \gamma^2) - \beta^2) = 9.97$ . With  $I = 136$  eV, the parenthesis is  $B = 5.06$  (this is called the *Bethe stopping number*). With  $I = 150$  eV, the parenthesis is  $B = 4.96$ , for a change of 2%, while the change in  $I$  is 10%. Thus small changes in  $I$  change  $M_1$  *very little*. For present purposes shell corrections etc are negligible.

moments  $M_\nu$  and  $\sigma_{tot}$  of Eq. (2) (notation of [7]) are calculated in the computations. Results of calculations of  $M_0$  and  $\sigma_{tot}$  for Ne are given (without the coeff.  $8\pi a_0^2 Ry/mv^2$ ) in Table 2, for Ar in Table 3. The fractional difference between  $M_0$  and  $\sigma_{tot}$  in percent is given as “diff%”.

Table 2. Comparison of  $M_0$  for Ne calculated with FVP and  $\sigma_{tot}$  calculated with Eq.(2) (using  $\mathcal{J}_1 - \mathcal{J}_2 = 2.852$ ).

$T(\text{MeV})$	$M_0$	$\sigma_{tot}$	diff%
10	13.59	11.89	14.3
30	15.65	13.93	12.3
100	17.81	16.06	11.1
300	19.69	17.87	10.2
500	20.58	18.73	9.9
1000	21.95	20.05	9.5
3000	24.76	22.81	8.5
10000	28.66	26.70	7.3
30000	32.57	30.67	6.2

Table 3. Same as Table 2 for Ar using  $\mathcal{J}_1 - \mathcal{J}_2 = 4.268$ .

$T(\text{MeV})$	$M_0$	$\sigma_{tot}$	diff%
10	34.56	31.02	11.4
30	39.37	35.82	9.9
100	44.40	40.85	8.7
300	48.68	45.13	7.9
500	50.70	47.15	7.5
1000	53.81	50.26	7.1
3000	60.31	56.77	6.2
10000	69.40	65.96	5.2
30000	78.01	75.30	3.6

We see that a similar difference occurs for  $M_0$  for Ne and Ar as for Si.

The stopping power  $M_1$  for both gases calculated with FVP differs by less than 1% from ICRU, or from the value calculated with Eq.(6).

## 4 Conclusions

Whenever the GOS approximation shown in Fig. 1 is used, e.g. in GEANT 4 or in PENELOPE, we must expect that  $M_0$  will be inaccurate. Since the important quantity for the estimates given in Tables 2 and 3 is  $(\mathcal{J}_1 - \mathcal{J}_2)$  used in Eq. (4), the differences depend strongly on it. An extensive list is given in [9]. In principle the same must be said for  $S(-1)$ , but these values are self-consistent and based on new experimental data for  $f(E; 0)$  [13, 14] used in programs BethNe.for and BethAr.for.

Since the difference in  $M_0$  is related to the differences in the CCS seen in Fig. 5 of [2], there is no simple correction that can be applied to the FVP-CCS. While a correction of  $M_0$  by using Eq. (2) would correct the straggling function for the number of collisions (Poisson term in Eq. (2) of [2]), it would not produce the correct shape for the energy loss straggling function, Fig. A.1 in [2].

It must be noted that for *electrons* the angular distributions of secondary electrons will depend on the shape of the GOS functions (Seth Hoedl, private communication, Dec. 2008).

## References

- [1] *Comparison of B-F and FVP inelastic collision cross sections*, Hans Bichsel, will be posted at website:  
  
<http://faculty.washington.edu/hbichsel/>
- [2] *A method to improve tracking and particle identification in TPCs and silicon detectors*, Hans Bichsel, Nucl. Instr. and Meth. **A 562** (2006) 154-197.
- [3] *Calculation of inner-shell ionization ...*, D. Bote and Fancesc Salvat, Phys. Rev. A **77** (2008) 042701
- [4] *Straggling in thin silicon detectors*. Hans Bichsel, Rev. Mod. Phys. **60** (1988) 663.
- [5] Manson, ST. (1972). Inelastic collisions of fast charged particles with atoms: ionization of the aluminum L shell, Phys. Rev. **A 6**, 1013-1024.

- [6] Walske, M.C. *The stopping power of K-electrons*, Phys. Rev. **88** (1952) 1283-1289, and *Stopping power of L-electrons*, Phys. Rev. **101** (1956) 940-944.
- [7] R. P. Saxon, Phys. Rev. A **8** (1973) 839.
- [8] Inokuti, M. (1971). Inelastic collisions of fast charged particles with atoms and molecules- the Bethe theory revisited. Rev. Mod. Phys. **43**, 297-347, and **50**, 23 (1978).
- [9] M Inokuti, R P Saxon and J. L. Dehmer, Int J Radiat Phys Chem **7** (1975) 109
- [10] M Inokuti and Y-K Kim and R L Platzman Phys Rev **164** (1967) 55
- [11] *Approximation methods to calculate straggling functions* H. Bichsel, Nucl. Inst. Meth. **A 565** (2006) 1-8.
- [12] *Penetration of protons, alpha particles and mesons*. U. Fano, Ann. Rev. Nucl Sci. **13** (1963) 1-66.
- [13] *Atomic and molecular photo absorption*. Joseph Berkowitz, Academic Press ( A division of Harcourt) 2002.
- [14] *Mean excitation energies for the stopping power of atoms...* S. Kamakura, N. Sakamoto et al., J. Appl. Phys. **100** (2006) 064905.